

PROGRESS TOWARDS AN INDUSTRY-FRIENDLY LES CAPABILITY

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Overview

- Paper objective
- Why higher order ?
- ► The BOXER Environment & LES/HOTnewt
- Turbomachinery & aerospace examples
- Computer resources
- Post-processing
- Summary

Paper objective

- Our objective is not to show LES and compare with experiment
 - lots of people do that
- Our objective is to show affordable LES which any engineer might perform at their desk
- This is delivered by a combination of novel software & hardware



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Why higher order?

- There is widespread misunderstanding about the role & advantages of higher order methods
- ► The key measure of the usefulness of a simulation is the level of computer resource needed, in simple terms:
 - the power in kWh and elapsed wall-clock time needed to perform a simulation in which the appropriate physical space & time scales are successfully resolved
- Clearly higher order methods deliver higher accuracy than lower order methods on the same mesh but with more floating point operations needed to attain that accuracy
 - so the key question really is: which approach uses less resource:

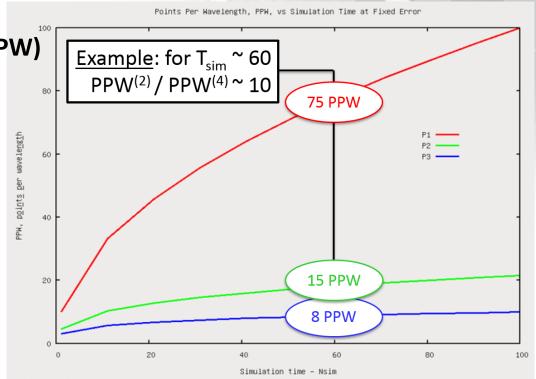
a low order method on a finer mesh or a high order method on a coarser mesh?



Higher Order Simulation Methods - PPW [Leland Jameson, 2001]

Points Per Wavelength (PPW)

- The figure illustrates this trend for P1, P2 & P3...
- ► This shows that a low order P1 method ("second order") might need a factor of 10 more PPW in 1D than a P3 method ("fourth order") – in 3D this becomes an astonishing factor of 1000!

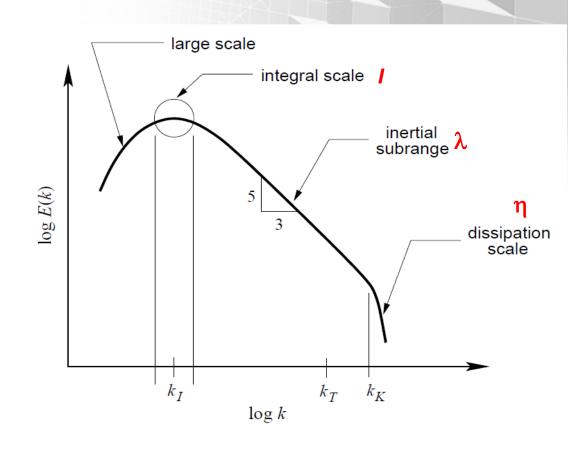


Simulation time T_{sim} for fixed E_{sim}

Hence, provided the higher order method does not consume too much extra memory per DOF, or too many extra floating point operations, then a welldesigned algorithm would permit a better computer memory – wall-clock performance

Turbulence scales & the energy spectrum

- There are several scales
 - the Integral scale (or "outer" scale), I
 [commonly the scale is defined as I ~ 0.1 L where L is the scale of the flow domain]
 - the Taylor microscale within the inertial subrange, λ
 - the **Kolmogorov** (or "inner" scale), η



Turbulence energy wavenumber spectrum

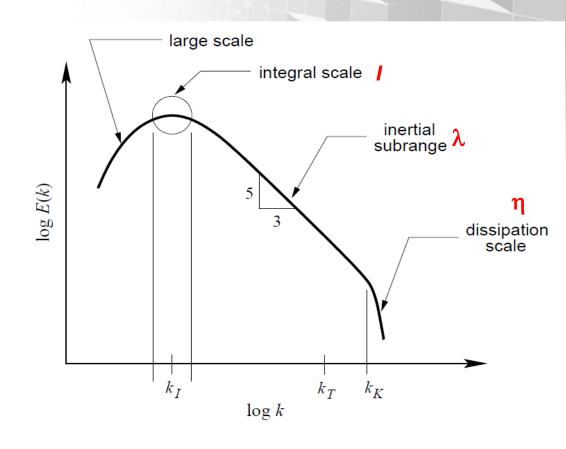


Turbulence scales & the energy spectrum

- These scales are related by:
 - $\eta / I \sim Re_I^{-3/4}$
 - $\lambda / I \sim Re_I^{-1/2}$

where $Re_I = |u'|I/v$ is the "turbulent Reynolds number"

- Hence in terms of wavenumber:
 - Taylor scales: $k_T \sim k_I Re_I^{+1/2}$
 - Kolmogorov : **k**_K ~ **k**_I Re_I +3/4



Turbulence energy wavenumber spectrum



Example: LES resolution requirements

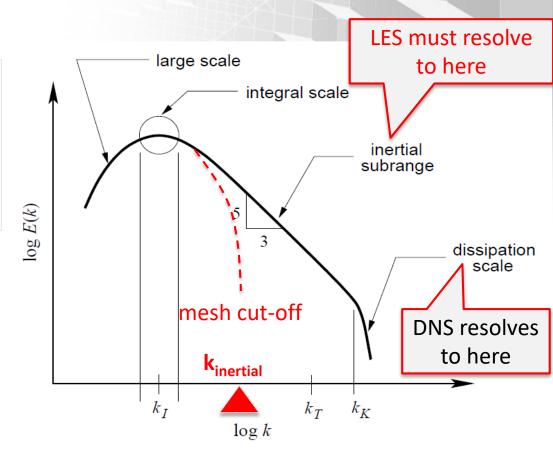
Example:

- Consider a LxLxL 3D domain with L=0.1m and Re₁=10⁺⁶
- then with I = 0.1Land (say) |u'| = 10%Uso that $Re_I = 10^{+4}$
- Hence

Integral scale: $k_I \approx 314$. Taylor scale: $k_T \approx 31400$.

 SO define a target wavenumber in the inertial subrange

 $k_{inertial} \sim 3140$.



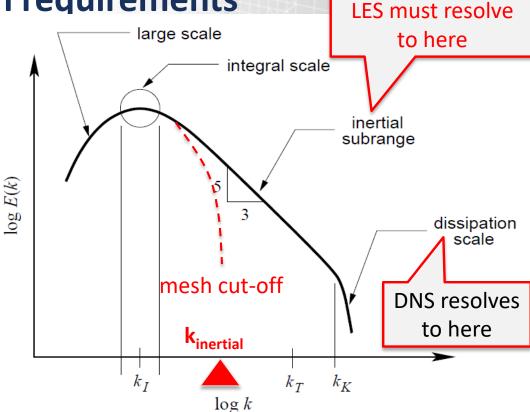


Example: LES resolution requirements

 The Table shows the mesh sizes that would be needed to resolve to the target wavenumber

 $k_{inertial} \sim 3140$.

 Also shown are the total Degrees of Freedom (DOF) and an estimate of the floating point operations needed (from our own code – HOTnewt)



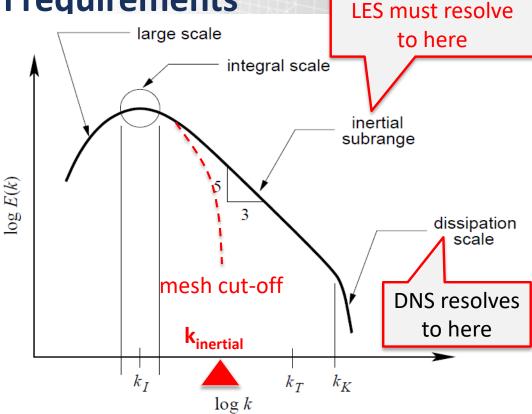
Order	DOF/cell	PPW	Mesh size (B)	Relative size	DOF (B)	Floats/∆t/ mesh cell	Relative floats
P1	8	75	421.	1	16840.	$3.6x10^3$	1
P2	27	15	3.3	0.0078	445.	$6.9x10^3$	1.94
Р3	64	8	0.51	0.0012	163.	14.7x10 ³	4.09

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Example: relative cost

► The difference in mesh size is astonishing – but of course higher order methods consume more floats per cell to achieve the higher accuracy – so if we define the *Relative Cost = relative mesh size x relative floats* we see:

Order	Relative Cost
P1	1
P2	0.015 = 1/ 66.2
P3	0.0049 = 1/203.

- ► The potential reduced Relative Cost which translates directly into reduced computer energy requirements — derived from higher order methods is astonishing — and, as we'll see, the key to unlocking their potential is being able to develop a sufficiently coarse, higher order mesh
- This has strong implications for the energy cost of the simulation roughly
 1 Gflop needs 1 Amp!



Example: relative cost

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Order	Relative Cost			
P1	1			
P2	0.01 <mark>5 = 1/66.2</mark>			
P3	0.0049 = 1/ 203 .			

- ➤ The potential reduced Relative Cost which translates directly into reduced computer energy requirements derived from higher order methods is astonishing and, as we'll see, the key to unlocking their potential is being able to develop a sufficiently coarse, higher order mesh
- This has strong implications for the energy cost of the simulation roughly
 1 Gflop needs 1 Amp!



Higher Order Simulation Methods

- So, given the apparent overwhelming advantages of higher order methods, why are they not in use in industry?
- ► The key issues are implementing these methods on real-world, realistic meshes which usually are hybrid, consisting of hexahedra, tetrahedral, prisms & pyramids, since this is the only meshing style which can be automated and can be applied to complex industrial geometries

AND integrating the high order method within a process chain giving access at one end to higher order geometry – for higher order meshes – and then at the other end higher order post-processing

- Hence: the BOXER Environment & HOTnewt
 - see AIAA 2015-0833, AIAA 2016-0555, AIAA 2017-0742,...



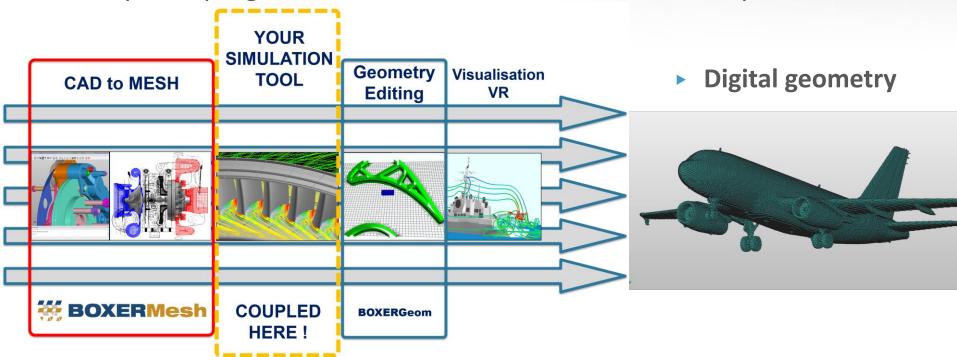
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BOXER Environment



- Supports an End-to-End Parallel Simulation Environment
 - Built on Digital Geometry
 - Fully scalable
 - Written with the flexibility to leverage future HPC & distributed parallel computing
- Very closely aligned with NASA's 2030 vision for revolutionary CFD



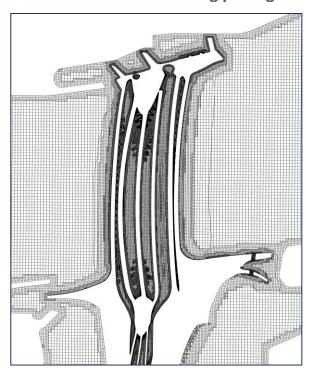


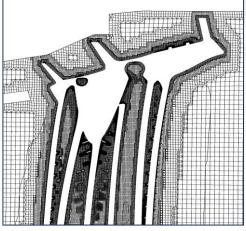


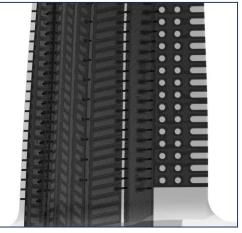
BOXERMesh – Complex geometry

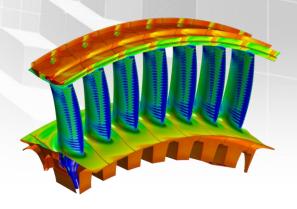
 An HP turbine rotor including cooling air system, shroud and under-hub

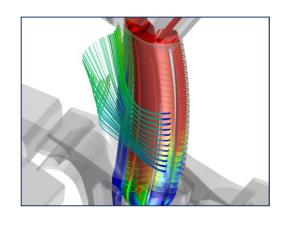
Mesh of the main gas path and cooling passages













BOXERMesh – Multi-region

 Fluid and solid phases are meshed simultaneously and with conformal interfaces

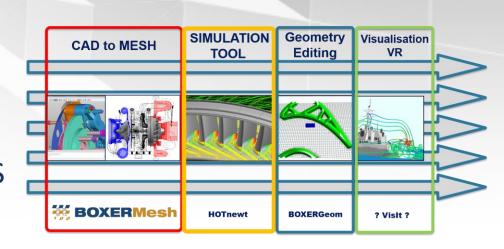




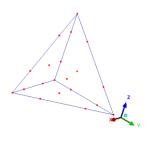


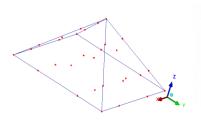
CFD SOLVERS HOTnewt

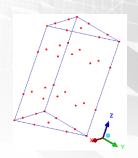
Fast, efficient higher-order LES

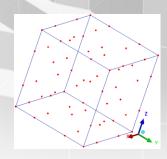


HOTnewt - next generation LES flow solver







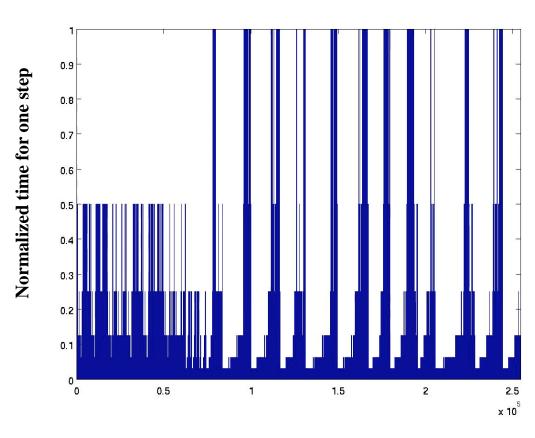


- Practical: runs on full hybrid unstructured (Boxer) meshes
- <u>Efficient</u>: Explicit approach using MPI+OpenMP low memory footprint ideal for many-core / coprocessor systems (like the Intel PHI.....)
- ► <u>Fast</u>: time-accurate local time-stepping giving potential speed-up of 10 to 100x relative to conventional (uniform time step) algorithms **novel STEFR scheme**
 - Local space-time-extension for time marching, local Flux Reconstruction for space (based on Huynh [2007])
 - Low-memory: as low as 32Gb / Mcell in 3rd order, wall resolved
 - Wall-resolved or wall-modelled (implicit sub-grid model based on Park & Moin [2014])
 - Quadrature-free, differential form, no mass matrix
 - Up to 4th order accurate in space



Space Time Extension of FR (STEFR)

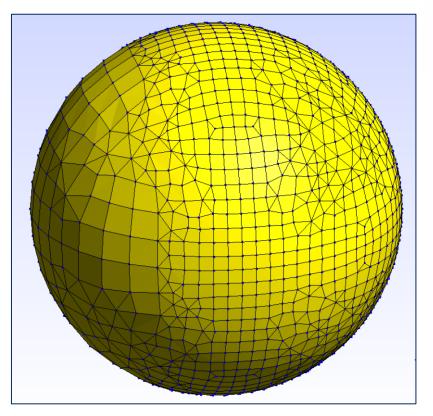
- We use local time stepping within the framework of a special time integration which preserves time accuracy
 - For each time step in the larger cells many steps are taken in the smaller cells
 - The main challenge is maintaining an efficient parallel load balance
- This has the potential to be 10~100 times faster on hybrid meshes for realistic industrial-class problems than classic, explicit timemarching (eg. R-K)

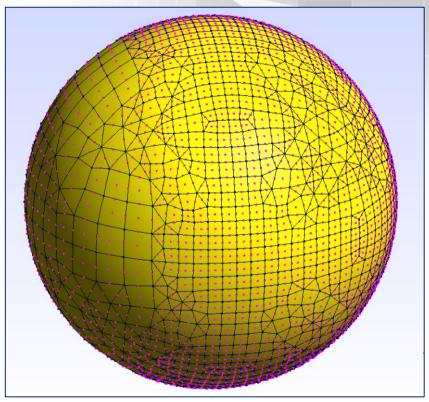


Elem id



HOTnewt - Flow past a sphere

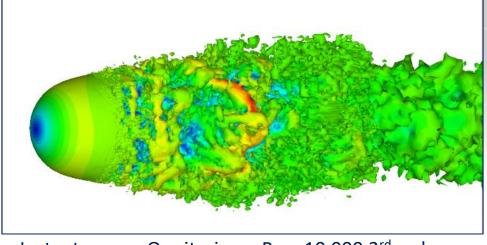




Benefit of higher-order geometry: higher fidelity representation at equal or lower cell count

HOTnewt – Higher order improves accuracy for same cost

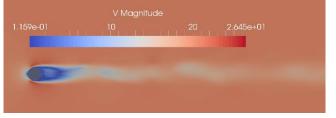
- Flow past a sphere at Re=300 & Re=10,000
- Calculated 2nd, 3rd and 4th order runs of similar computational cost
 - Increased order <u>reduces</u> mesh cell count & DoFs

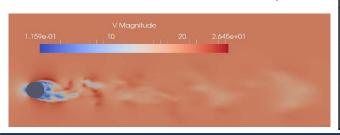


Instantaneous Q-criterion – Re = 10,000 3rd order



$$Re = 300$$

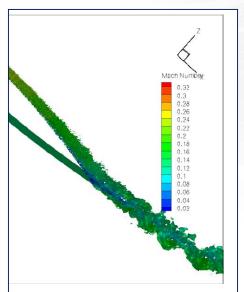


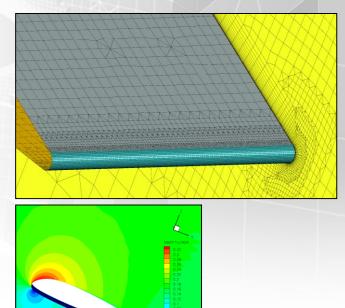


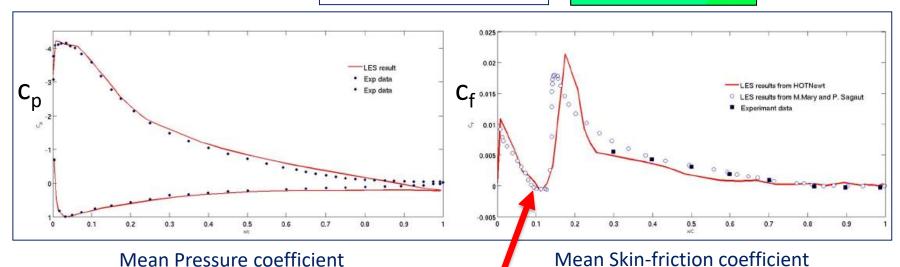
Reynolds number	Order of accuracy	Ncells	Ndofs	Cd	Cd (combined calc & expt)
300	2 nd	419250	13.9M	0.676	
300	3 rd	155286	15.2M	0.664	
300	4 th	52447	10.7M	0.658	0.657
10000	2 nd	3783863	135.3M	0.448	
10000	3 rd	735883	79.2M	0.439	
10000	4 th	164013	37.7M	0.429	0.416

HOTnewt – LES for an airfoil

- Standard airfoil
- Re = 2.1 x 10⁶ and α=13.3°; span = 3% of chord
- 2nd order with local 3rd order p-refinement –
 15.2M DoF
- ▶ wall-resolved Y⁺ ~ 1.3







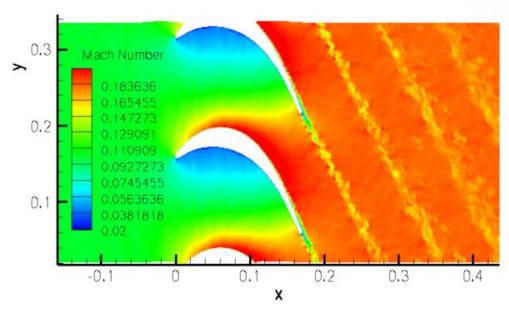
Wall-resolved HOTnewt LES predicts transition

CAMBRIDGE FLOW SOLUTIONS

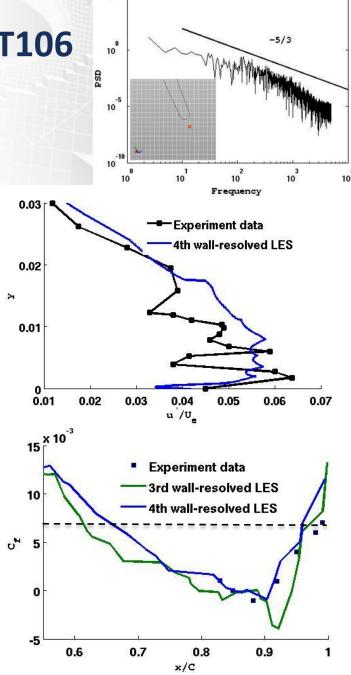
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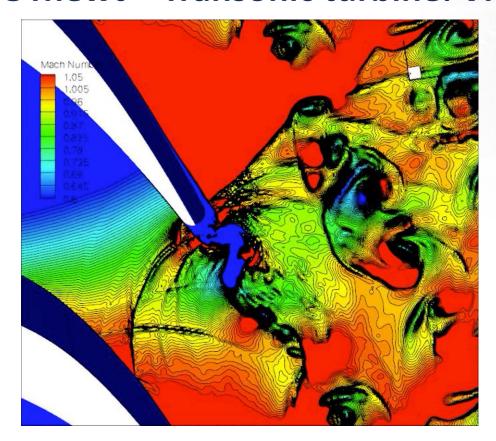
HOTnewt – Low pressure turbine: T106



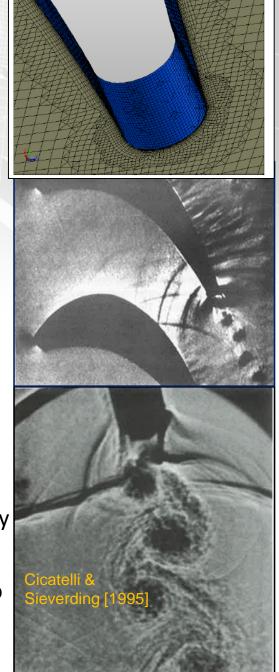
- ► Tested at the Whittle: suction side boundary layer transition & separation bubble
- Re= 1.1×10^5 ; Inlet Mach is 0.1
- Spanwise extent of the domain $L_z = 0.075C$
- STEFR speed-up ≈ 8.1 rel. to conventional, uniform time-stepping
- 4th order wall-resolved LES, 110k cells



HOTnewt – Transonic turbine: VKI



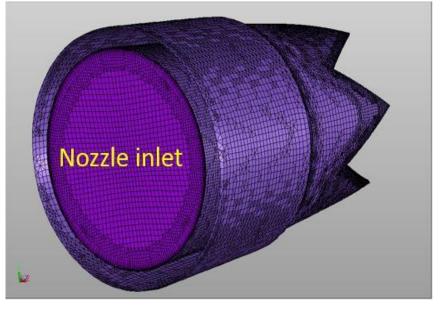
- Tested at the VKI: reflected shock at the suction side boundary layer interaction; shock-trailing edge vortex wake interactions
- Re= 8.5×10^5 , **3**rd **order**, STEFR speed-up of ~8.1 compared to conventional methods
- Wall-resolved LES, 107k cells, with 137.3M DOFs

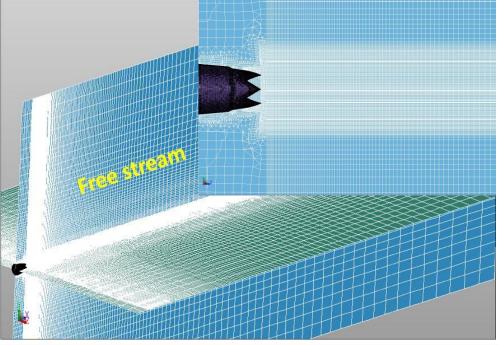


NASA Acoustic Reference Nozzle

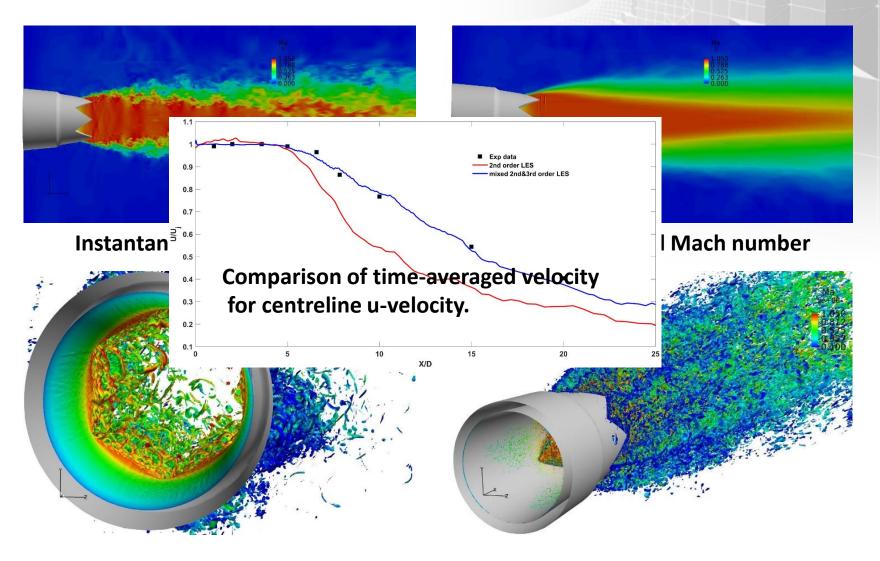
Geometry	Nozzle inlet total pressure p_0 (Pa)	Nozzle inlet total temperature $T_0(\mathbf{K})$	Free stream static pressure p_{∞} (Pa)	Free stream temperature $T_{\infty}(\mathbf{K})$
SMC001 nozzle	1.78×10^{5}	286.4	9.7×10^{4}	280.2

Case ID	Order of accuracy	Number of cells	Number of DOFs	Spee d Up Ratio	Number of nodes on our cluster	•	Memory consumption(Gb)	Wall- clock time for $1T_p$ (hours)
SMC001_1	2 nd	9.04M	338.4M	16.3	1 (8 PHI cards)	80	167	5.09
SMC001_2	mixed 2 nd /3 rd	7.66M	671.1M	29.2	4 (3 PHI cards each)	160	317.4	9.72





NASA Acoustic Reference Nozzle

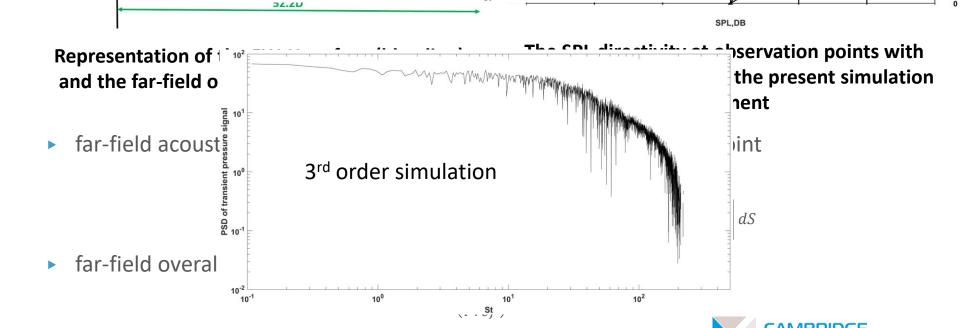


Snapshots of instantaneous Q-criterion illustrating the jet structure, coloured by Mach number



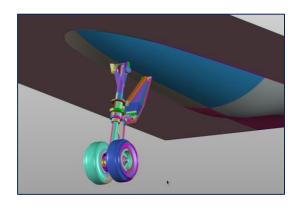
Acoustic post-processor: ffowcs Williams-Hawkings (FWH) integration

2nd order simulation

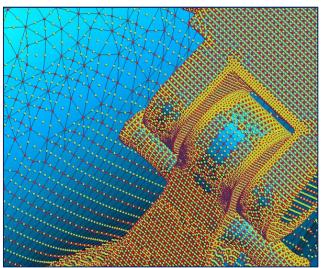


HOTNewt – Landing gear aero-acoustic case

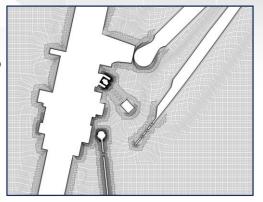
- ► BANC II Landing gear aero-acoustic test case
 - 3rd order, wall-modelled 11.1M cells 862 M DoFs
 - 301Gb memory running on 2,736 cores on "Ulysses", our new CFS 12kW
 Intel PHI cluster
 - Complete simulation in ~1 week
 - STEFR speed up is ~35 x faster than uniform time-step LES

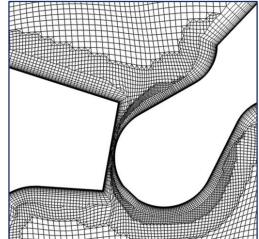


Landing gear geometry

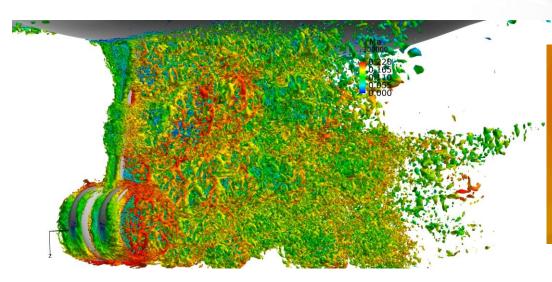


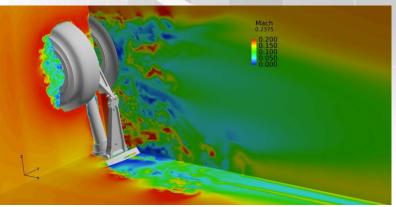
Detail of P2 mesh





HOTNewt – Landing gear aero-acoustic case





Mach contours ($M_{\infty} = 0.2375$)

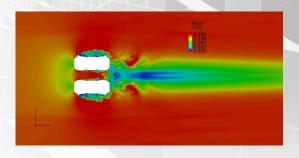
Instantaneous Q= 300,000

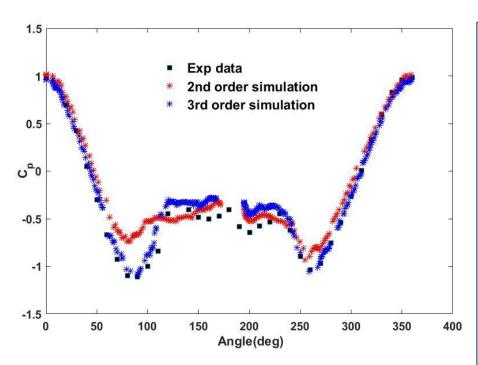
- Wall-modelled mesh: 3rd order
- ▶ 11.1M cells, 862M DOFs
- ▶ 18.7 wall-clock hours for one flow-past time, ΔT_p , based on strut size and run on "Ulysses" our 12kW Intel PHI system
- Complete simulation in ~ 1 week



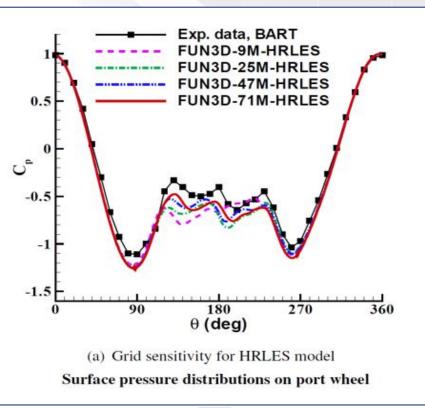
HOTNewt – Landing gear aero-acoustic case

- 3rd order result is better, with no overprediction relative to data
- Favourable comparison with NASA/FUN3d run on much finer meshes





HOTnewt 2nd & 3rd order C_p distribution around port wheel

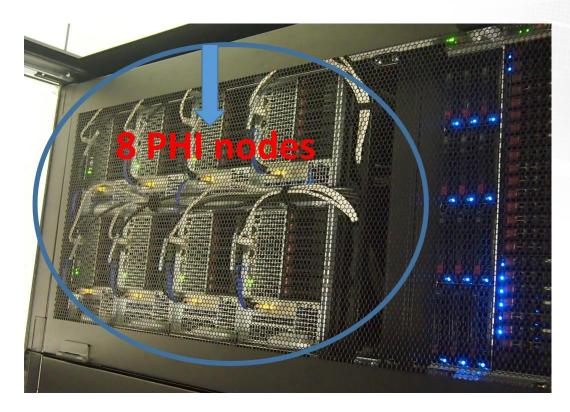




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CFS Intel Phi Cluster - our 12kW Intel PHI system



"Ulysses"

Architecture: 16 Intel Xeon E5-2692 8C, 48 Xeon PHI 31S1P cards.

Power: 12 KW

Memory: 1TB on CPUs and

384GB on PHI cards

Speed: ~30 TFLOPS

Cost: ~\$75k = \$0.075 milion

- Built using an Innovate UK SMART award, "<u>Ulysses</u>" is equivalent to about 600-800 conventional CPU cores depending on loading but a fraction of the cost compared to CPU cluster
- Equivalent to less than 1/10 the cost of a CPU-core-hour (Jaeggi [2016])
- Ideal for intensive simulations, low hardware & running cost



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Architecture: 32,000 Intel Xeon E5-2692 12C, 48,000 Xeon PHI 31S1P cards.

Power: 17.6 MW (24 MW

with cooling)

Memory: 1000TB on CPUs

and 375TB on PHI cards

Speed: 33.86 PFLOPS

Storage: 12.4PB

Cost: US\$390 million

"Ulysses" is equivalent to about to ~700 conventional CPU cores but consumes 12kW compared to ~192kW for ~700 CPU cores within Tian-he 2

factor x16 less electricity and x57 cheaper to buy!

HOTnewt is highly optimised to run on this type of architecture



- It is difficult to find comparative computer resource data in the open literature

 − and comparisons are made doubly difficult by the different mesh sizes and algorithms
- Khorrami [2015] does give data for the ONERA code CEDRE [2011] for the BANC test case
 - CEDRE was run as a second order solver with a 70M cell mesh on 480 conventional cpu cores and needed 1.44 hours per Δt_p
- ► The present *HOTnewt* simulations were
 - run 3rd order with 11.1M cells (862 M DoFs) wall-clock 18.7 hours of our 12kW Intel PHI system were needed for one flow passing period Δt_p
- Hence, the <u>raw comparison</u> is:
 - ► ONERA/CEDRE: 480cpu_1.44 (cores_wall clock hours/ $\Delta t_{P.}$)
 - ► HOTnewt: 48phi_18.7 (cores_wall clock hours/ Δt_p)
- BUT how do we allow for the different hardware, mesh size & order?



- Hardware:
 - our Intel PHI cluster benchmarks to be equivalent to ~700 conventional cpu cores so we can simply scale the *HOTnewt* simulations to 480 conventional cores
- Hence, the comparison <u>scaled for hardware</u> is:

► ONERA/CEDRE: $480_{1.44}$ (cores_wall clock hours/ Δt_{P})

► HOTnewt: $480_{27.3}$ (cores_wall clock hours/ Δt_p) [scaled hardware]

- On the face of it HOTnewt is therefore much slower than CEDRE...
- ...BUT the mesh size & order are different...



- Mesh size & order (1):
 - 70M cells in a second order solver is equivalent to (15/75)³x70M=0.55M cells in a third order solver using the PPW data from earlier
 - Scaling the computer work between meshes is partly the ratio of mesh sizes (this is simply the basic floating point work) but also the (ratio of mesh sizes)^{1/3} to approximately scale the time step change assumed limited by a CFL number criterion
- ► Hence, the comparison **scaled for hardware & mesh/order** is:

► ONERA/CEDRE: $480_{1.44}$ (cores_wall clock hours/ $\Delta t_{P.}$)

► HOTnewt: 480_0.49 (cores_wall clock hours/ $\Delta t_{P.}$) [scaled hardware, mesh size]

This indicates HOTnewt would be a factor 2.9 faster than ONERA/CEDRE



- Mesh size & order (2):
 - An alternative approximate scaling is to try to go the other way from 3rd order to 2nd order
 - The *HOTnewt* 11.1M cell 3rd order mesh is equivalent to a (75/15)³x11.1M =1,423M cell 2nd order mesh!
 - The run time for this would scale as (mesh size)4/3 as described above
- Hence, the comparison scaled for hardware & mesh/order is:
 - ▶ "2nd order solver": 480_**79.8** (cores_wall clock hours/ Δt_p) [scaled mesh size]
 - ► HOTnewt: $480_{27.3}$ (cores_wall clock hours/ Δt_{p}) [scaled hardware]
- ► This again indicates *HOTnewt* would be a factor 2.9 *faster* than a "2nd order solver"
 - when combined with the factor ~10 reduced energy consumption of our Intel PHI system *HOTnewt* LES would appear to be around a factor ~29 cheaper than other LES methods for comparable resolution.

Overview

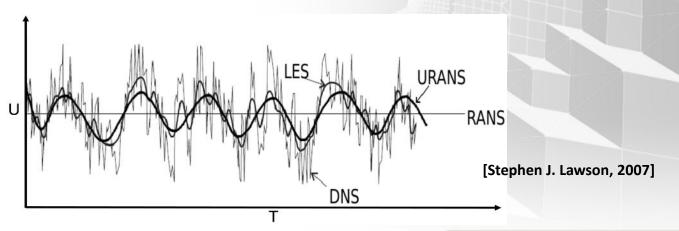
- ► Paper objective
- ► Why higher order ?
- ► The BOXER Environment & LES/HOTnewt
- ► Turbomachinery & aerospace examples
- Computer resources
- Post-processing
- Summary

Post-processing & "Big Data"

- The big challenge now is post-processing getting useful, sensible engineering data out of these large simulstions
- Certainly post-processing will need to be implemented in parallel, and close-coupled into to the solver parallel data structures
 - But there are other approaches which may well contribute
- ► The main flow information (low frequency, most energy-containing main industrially interesting statistics) could be efficiently reconstructed and analysed using low order orthogonal modal modes, which are remarkably fast and low memory
- On-the-fly POD data-extraction and analysis during the LES would allow these benefits to be achieved in huge, massively parallel Billon+ DOF simulations - suggesting that great efficiency in post-processing these "big data" problems is indeed achievable
 - Further, the connections between the low frequency part and high frequency part could be investigated further, case by case (high frequency part, turbulence, unsteadiness, ...) to drive insight into improved low-order modelling like RANS...



Hierarchical Proper Orthogonal Decomposition (HPOD)



Examples of time signals from DNS, LES, URANS and RANS simulations

Review of Karhunen-Loeve Decomposition (KLD) met

$$U(x,t) = U_m + \sum_{i=i}^{N_t} c_i(t) \Phi_i(x)$$

Huge memory consumption for massive high fidelity unsteady results

▶ $N_t \le N$ is the selected number of rapshots for reconstruction

$$\boldsymbol{B} = (1/N)(\boldsymbol{A}^T\boldsymbol{A}), \boldsymbol{A}$$
 denote an $M \times N$ matrix of real data

$$\mathbf{B}v_i = \lambda_i v_i, \quad \text{for } i \in [1, N], \lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_N > 0$$

$$\Phi_i = \frac{1}{\sqrt{\lambda_i}} \sum_{j=1}^{N} (v_i)_j U_j^h, \quad for \ i \in [1, d]$$



Multi-level orthogonal modal decomposition – on-the-fly

- ► The analysis is re-cast so that it can be performed on-the-fly closely integrated into the flow solver data structures
- Orthogonal modal solution

$$u_{i,j}^m = \int_E \phi_j^m U_i dE, \qquad j \in [1, N_{dofs}^m]$$

where $\int_{E} \phi_{i}^{m} \phi_{j}^{m} dE = vI$

Order of accuracy	1 st	2 nd	3 rd	4 th
Number of DOFs	1	4	10	20
Size ratio of \boldsymbol{A} with same number of snapshots	1	4	10	20

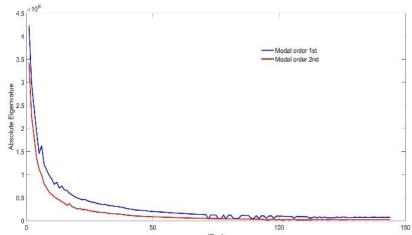
▶ The reconstruction of flow variables on a nodal point \vec{p} on i —th element is

$$u_i^n(\vec{p}) = \sum_j^{N_{dofs}^m} \phi_j^m(\vec{p}) u_{i,j}^m$$

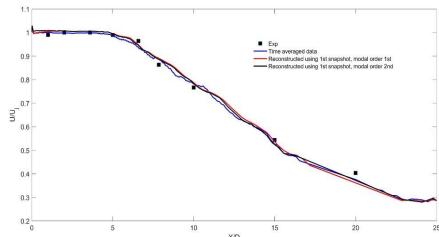


HPOD analysis for SMC001 transonic nozzle case

Job ID	Modal order	No. of variables per cell	Total DOFs	Size of instantaneous results (Gb)	No. of snapshots	Size of matrix A(single precision, Gb)	Actual memory consuming for HPOD(Gb)	Size of modal result for each snapshot(Gb)
	1 st	1	7665463	1543.5	250	7.14	8.35	0.1591
	2 nd	1	30661852	1543.5	250	28.56	28.37	0.6364
	3 rd	1	76654630	308.71	100	28.56		1.591
	1 st	3	22996389	1543.5	250	21.42	21.3	0.4773
	2 st	3	91985556	1543.5	250	85.68	85.2	1.9092
	3 rd	3	2.3×10^{8}	308.71	100	85.68		4.773



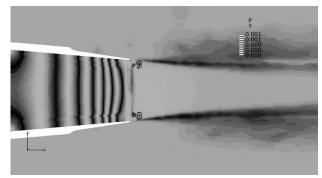
Plot of Eigenvalues(not including 1st mode) from the HPOD analysis



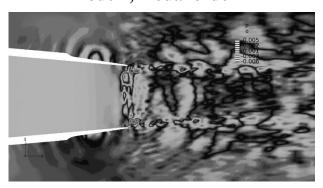
Comparison of reconstructed, time-averaged centreline uvelocity using the 1st POD mode



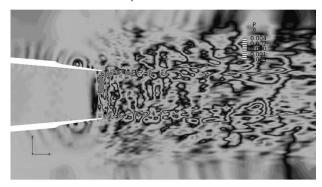
POD modes of pressure field in the X-Z plane (Y=0)



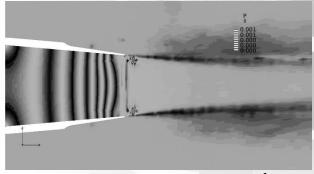
mode 1, modal order 1st



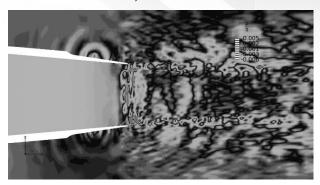
mode 2, modal order 1st



mode 9, modal order 1st



mode 1, modal order 2nd

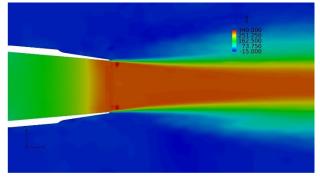


mode 2, modal order 2nd

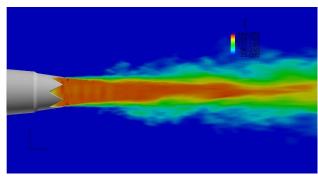


mode 9, modal order 2nd CAMBRIDGE

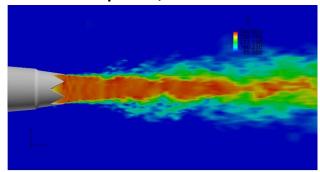
Reconstruction of velocity field in the X-Z plane (Y=0)



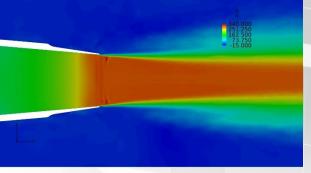
Reconstructed u using mode 1 order 1st



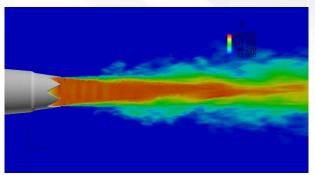
15th snapshots, modal order 1st



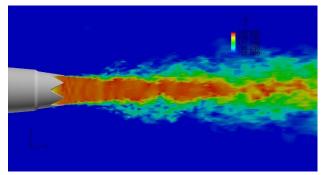
145th snapshots, modal order 1st



Reconstructed u using mode 1 order 2^{nd}



15th snapshot, modal order 2nd

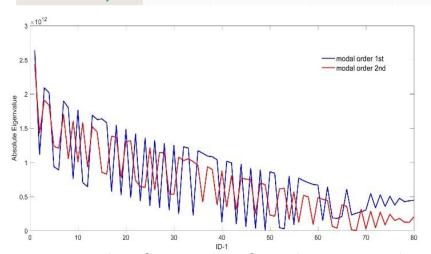


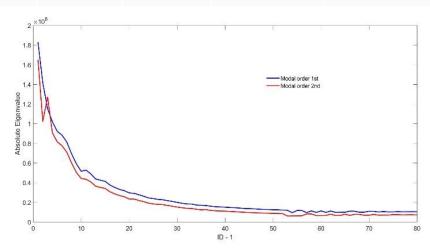
145th snapshot, modal order 2nd



HPOD analysis for Landing Gear case

	_							
Job ID	Mod al order	No. of variables per cell	Total DOFs	Size of instanenous results (Gb)	No. of snapshops	Size of matrix A(single precision)	Actual memory consuming for HPOD (Gb)	Size of modal result for each snapshot (Gb)
Landing-gear-KO- Pressure	1 st	1	14649682	2286.86	250	13.65	20.1	0.304
Landing-gear - K1-Pressure	2 nd	1	58598728	2286.86	250	54.6	59.86	1.216
Landing-gear - K2-Pressure	3 rd	1	14649682 0	457.37	100	54.6		3.04
Landing-gear - KO-Velocity	1 st	3	43949046	2286.86	250	40.95	45.8	0.912
Landing-gear - K1-Velocity	2 st	3	1.76×10^{8}	2286.86	250	163.8	169.1	3.648
Landing-gear - K2-Velocity	3 rd	3	4.4×10^{8}	457.37	100	163.8		9.12

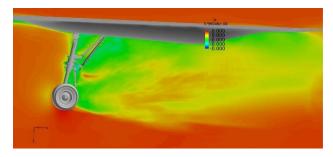




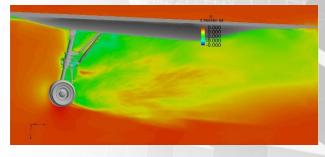
Plot of Eigenvalues from the HPOD analysis: (left) for pressure and (right) for velocity



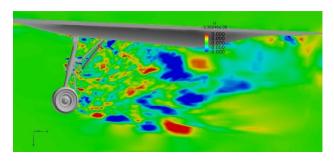
POD modes in the X-Z plane (Y=0) for velocity u-component



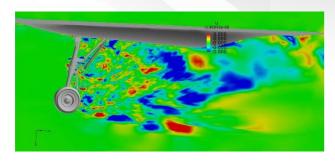
mode 1, modal order 1st



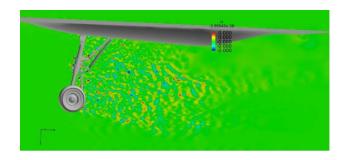
mode 1, modal order 2nd



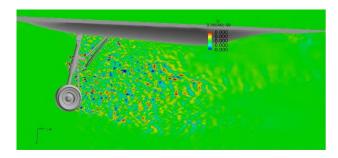
mode 2, modal order 1st



mode 2, modal order 2nd



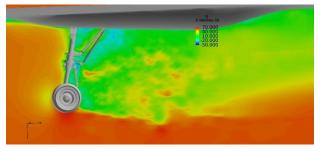
mode 10, modal order 1st



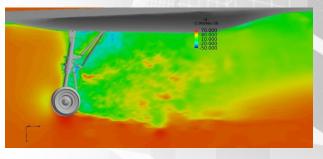
mode 10, modal order 2nd



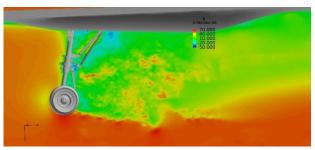
Reconstructed velocity u-component in the X-Z plane (Y=0)



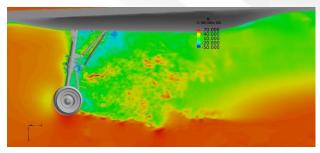
5th snapshots, modal order 1st



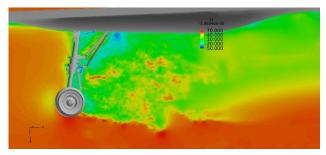
snapshot, modal order 2nd



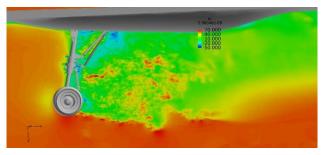
15th snapshots, modal order 1st



 15^{th} snapshot, modal order 2^{nd}



81th snapshots, modal order 1st



81th snapshot, modal order 2nd



Overview

- ► Paper objective
- ► Why higher order ?
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- ► Turbomachinery & aerospace examples
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Summary

- Our objective was not to show LES and compare with experiment
 - lots of people do that...
- Our objective is to show affordable LES which any engineer might perform at their desk
- We have demonstrated LES with acceptable accuracy on some turbomachinery/aerospace applications
- We have demonstrated that useful LES can be performed with significant reductions in computer resource cost
 - the key to unlocking this potential is being able to develop a sufficiently coarse, higher order mesh.
- We have shown the start of our response to the "big data" post-processing challenge in the form of on-the fly POD





Higher Order Simulation Methods – PPW

- The key is to understand mesh resolution
 - LES is unsteady and needs much greater mesh resolution than that required merely for a steady approximation
 - this resolution requirement increases as the simulation time increases...
 - mesh resolution is measured in terms of *Points Per Wavelength* (PPW)
- For any numerical scheme the Truncation Error (TE) for convection is of order

$$\Delta x^{p-1} \partial^p u / \partial x^p$$

where p depends on the scheme (2 for a P1 method, 3 for a P2 etc.)

In terms of harmonics $\mathbf{u} \sim \Sigma \mathbf{e}^{i\mathbf{k}\mathbf{x}}$ so for a typical wavenumber, $\mathbf{k} = 2\pi/\lambda$, the order of magnitude of the truncation error, TE, is

TE
$$\sim \Delta x^{p-1} k^p$$



Higher Order Simulation Methods – PPW

▶ If the simulation takes place over a time T_{sim} then the **total error** for that wave number is of order

$$E_{sim} \sim T_{sim} \Delta x^{p-1} k^p$$

If N_{sim} is the number of time steps and $\Delta t/\Delta x$ is constant then $T_{sim} \sim N_{sim} \Delta x$ then the

Points Per Wavelength, $\lambda/\Delta x$, is given by

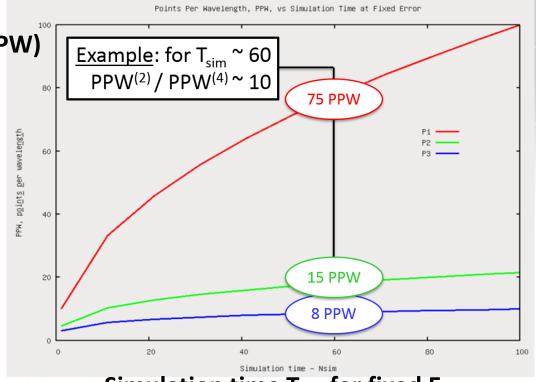
PPW
$$\sim (N_{sim}/E_{sim})^{1/p}$$



Higher Order Simulation Methods – PPW

Points Per Wavelength (PPW)

- The figure illustrates this trend for P1, P2 & P3...
- ► This shows that a low order P1 method ("second order") might need a factor of 10 more PPW in 1D than a P3 method ("fourth order") in 3D this becomes an astonishing factor of 1000!



Simulation time T_{sim} for fixed E_{sim}

- Since PPW and the associated DOFs (Degrees of Freedom) translate directly to computer memory, RAM, requirement then
 - provided the higher order method not consume too much extra memory per DOF then a well-designed algorithm could permit a better computer memory job size trade-off.

Higher Order Simulation Methods – Floats

- What happens to the operation count the computer run-time cost?
- Consider a basic <u>second</u> and <u>fourth</u> order convection operator:

$$Q_x^{(2)} = \frac{1}{2\Delta x}(u_{i+1} - u_{i-1})$$

$$Q_x^{(4)} = \frac{2}{3\Delta x}(u_{i+1} - u_{i-1}) - \frac{1}{12\Delta x}(u_{i+2} - u_{i-2})$$

In terms of operations $ops^{(2)} = 3 \& ops^{(4)} = 7$ if the coefficients $(1/2\Delta x \text{ etc.})$ are recomputed each use (to save memory)



Higher Order Simulation Methods – Floats

- So, the fourth order method needs more floats BUT for an unsteady simulation, for a given Fourier mode, the second order method needs far more Points per Wavelength
 - for example **PPW**⁽²⁾ / **PPW**⁽⁴⁾ ~ **10** in 1D
- Hence the relative cost in terms of arithmetic operations of a second order method compared to a fourth order one for the same accuracy in 3D is:

```
floats^{(2)}/floats^{(4)} \sim [(ops^{(2)}/ops^{(4)}) \times (PPW^{(2)}/PPW^{(4)})]^3 \sim 78!
```

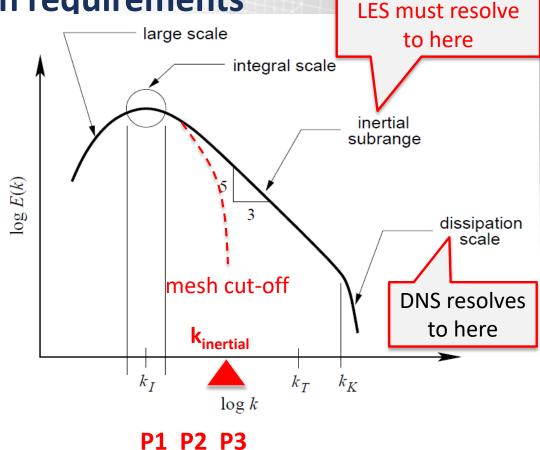
- Thus although the fourth order method needs more operations per DOF this is more than offset by the much reduced number of DOFs for a given accuracy leading potentially to orders of magnitude fewer computer operations – in 3D
- This has strong implications for the energy cost of the simulation
 roughly 1 Gflop needs 1 Amp!



Example: LES resolution requirements

 Consider a mesh with 100M cells – the maximum wavenumber which can be resolved is:

Order	Max. wavenumber on 100M cells
P1 = second	386.
P2 = third	1932.
P3 = fourth	3623.



Only the *fourth* order method can resolve into the inertial subrange!





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